



Flame Lift-Off Found to Affect the Evolution of Soot in Diesel Fuel Jets

Recent research suggests that partial premixing of fuel and air upstream of the flame lift-off location affects soot formation in a diesel fuel jet. Dennis Siebers, Brian Higgins, and Lyle Pickett recently investigated the effects of various diesel engine parameters on flame lift-off and the relationship between flame lift-off and soot formation in a diesel fuel jet. The research, part of Cooperative Research and Development Agreements with the automotive and diesel engine industries, was supported by DOE's Offices of Heavy-Duty Vehicle Technologies and Advanced Automotive Technologies.

The work was carried out in the CRF's optically accessible diesel combustion simulation facility using an electronically controlled, common-rail diesel fuel injector. Injection pressure, orifice diameter, and in-cylinder gas temperature, density, and oxygen concentration were among the parameters considered. (Oxygen concentration in an engine is affected by the amount of exhaust gas recirculation used.)

Images of OH chemiluminescence were used to measure flame lift-off length. OH chemiluminescence marks regions of high temperature combustion, such as occurs at the lift-off length. The distance between the injector orifice and the most upstream location of OH chemiluminescence on the fuel jet in the images was defined as the lift-off length. The effect of temperature on lift-off length is shown in Figure 1. The images show that as temperature increases, lift-off length decreases. The temperature trend is caused by an

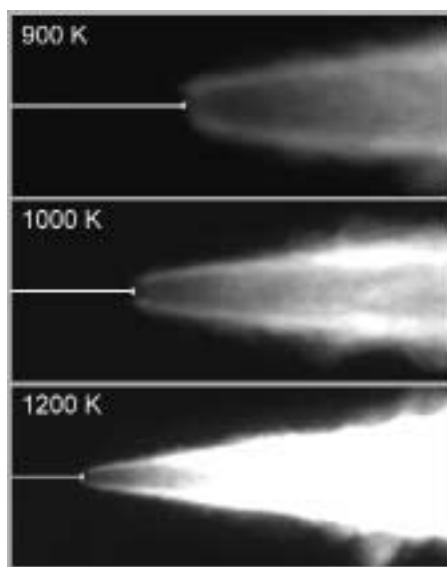


Figure 1. Time-averaged images of OH chemiluminescence for three different in-cylinder gas temperatures. The white line extending from the injector at the left edge indicates the lift-off length. Recent research suggests that the flame lift-off length can influence soot formation in a diesel fuel jet. The orifice diameter, pressure drop across the injector orifice, and in-cylinder gas oxygen concentration were 180 mm, 138 MPa, and 21%, respectively.

increase in flame speed with increasing temperature, which allows the flame to stabilize closer to the injector.

The data also showed that lift-off length increased with decreasing oxygen concentration and density and increasing injection pressure and orifice diameter. The trend with respect to injection pressure is the same as has been noted for atmospheric-pressure gas jets, while the trend with respect to orifice diameter is different than that observed for atmospheric-pressure gas jets. Atmospheric pressure jets typically show no lift-off length dependence on

orifice diameter. It is believed that fuel vaporization processes cause the orifice-diameter effect on lift-off on diesel fuel jets.

Total soot incandescence measurements (a relative indication of the total amount of soot formed) were made simultaneously with each lift-off length measurement to explore the link between soot formation and the degree of fuel-air premixing upstream of the lift-off length. The dominant trend shown by the data is that as the air entrainment upstream of the lift-off length increases, the soot incandescence (i.e., the amount of soot formed) decreases and approaches zero as the cross-sectional average equivalence ratio at the lift-off length in the fuel jet approaches two. This is true for a wide range of conditions. The disappearance of soot at a cross-sectional average equivalence ratio of two generally agrees with what is found in investigations of soot formation under completely premixed conditions. Under premixed conditions, typical hydrocarbon fuels do not produce soot for equivalence ratios less than approximately two.

Overall, the results show that there is a strong link between partial premixing of fuel and air upstream of the lift-off length and soot formation in diesel fuel jets. Current research is focusing on understanding this link and how various engine and injector parameters effect it in more detail.

Solid State Sensors Tested for Monitoring Hydrogen in Industrial Processes

Chemical manufacturers and petroleum refiners use steam reforming to extract hydrogen (H_2) from methane, refinery off-gases, and other feedstocks. Extracting H_2 from hydrocarbons requires vast amounts of high-pressure steam, electricity, and natural gas. If there was a way to rapidly and cost effectively monitor H_2 content in the various process streams, control strategies to improve plant productivity and reduce environmental impact could be implemented. Anthony McDaniel and Dennis Morrison, along with collaborators from Pennsylvania State University, Air Products and Chemicals, Inc., and DCH Technology are developing solid-state devices to measure hydrogen concentrations in industrial process streams. Funded by the Department of Energy's Office of Industrial Technologies Sensor Cross-Cut program, this project aims to produce inexpensive, robust, sensing elements capable of surviving the chemical and thermal extremes of the industrial reforming environment.

Thin-films of palladium-metal alloys change their electrical properties in the presence of hydrogen, allowing them to operate as hydrogen sensors. However, surface-mediated processes, such as competitive reactions among adsorbates and catalyst poisoning, interfere with hydrogen uptake by the palladium-metal alloy and adversely affect sensor performance. Ongoing work at the CRF and Penn State is focused on understanding the failure modes of these devices under various chemical and physical stresses in



Figure 1. The magnified photograph of a chemiresistor chip fabricated at Penn State's Nanofabrication Facility clearly shows the fine lines of several palladium-alloy chemiresistors. These chemiresistors are candidates for hydrogen sensors in the extreme process environments of steam forming. Tests at the CRF are aimed at evaluating a variety of resistor lengths, configurations, nascent resistivities, and thicknesses, as well as alloy composition and morphology.

order to design more process-compatible structures.

The sensor chips under investigation were fabricated at Penn State's Nanofabrication Facility and analyzed at the CRF for response and functionality. Wafers are patterned with a variety of test structures using conventional contact-lithography and liftoff. The Figure 1 photograph of a typical chemiresistor chip reveals the fine lines that are the resistor elements. This device has 12 separate resistor elements that differ in line-width, shape, and nascent resistivity.

The electrical responses of three resistor circuits to a pulse of H_2 are shown in Figure 2. The response of three different resistor elements to the H_2 pulse at 373 K is shown in Figure 2a, while the response of the 1.5-k Ω , 1.6-mm resistor at three different surface temperatures is shown in Figure 2b. So far, researchers find that the ultimate sensitivity and response depends on the operating condition as well as the physical characteristics of the films themselves. Future efforts will investigate the effects of alloy composition, film morphology, and protective overlayers on device performance. The overlayers are placed on the devices to help them withstand the extreme operating conditions of industrial reforming environments.

In addition to the laboratory work, field trials have begun with DCH Technology's commercial sensing elements. Three sensors were installed at a preconditioned sample point in a hydrogen cogeneration facility operated by Air Products and Chemicals, Inc. in

Wilmington, CA. The H_2 sensors were installed along a remote sampling line, along with other analytical instruments used at the plant. The importance of having a widely distributed system of sensors was demonstrated when the DCH sensor at the feedstock inlet indicated an excursion that had doubled the hydrogen concentration.

The CRF News is published bimonthly by the Combustion Research Facility, Sandia National Laboratories, Livermore, California, 94551-0969.

Director: William J. McLean, Mail Stop 9054

Editor: Howard Lentzner, Email: hlentz@sandia.gov

Graphic Artist: Daniel Strong

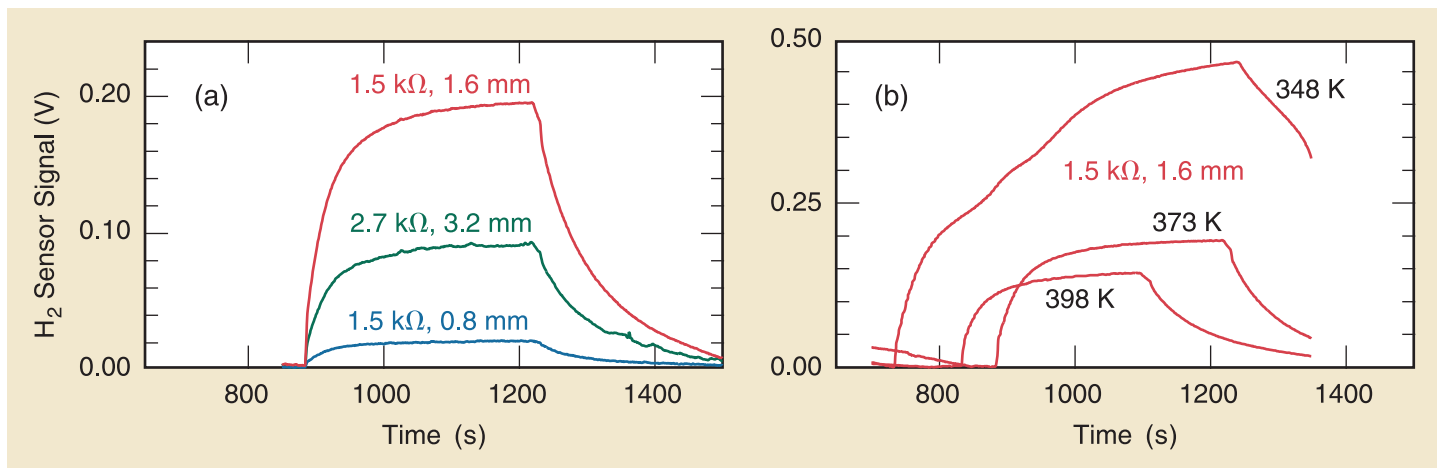


Figure 2. Plots of H_2 sensor signals with time for three different Pd-alloy resistors at 373 K (a) and for three different temperatures for the 1.5 k Ω , 1.6-mm-wide resistor (b). The curves show the dependence of sensor response to the width, nascent resistivity, and temperature of the resistor.

Periodically Twinned GaAs Crystals Yield Tunable, Long-Wavelength Infrared Laser Beam

In a recent collaboration between Sandia National Laboratories and Stanford University, a new nonlinear optical crystal was used to generate tunable long-wave ($\sim 8\text{--}12\ \mu\text{m}$) infrared (LWIR) radiation. The work performed by Tom Kulp and Scott Bisson and Ofer Levi, Loren Eyres, Thierry Pinguet, and Marty Fejer of Stanford, marks a major advance in the development of tunable continuous-wave (cw) LWIR laser sources. Broadly tunable LWIR lasers are needed for use in molecular absorption measurements because most organic molecules absorb at mid- and long-wave length distinct infrared frequencies related to their skeletal structure.

The new crystal, periodically twinned gallium arsenide (PTGaAs) was developed at Stanford and is being adapted for chemical sensing through the Stanford/Sandia collaboration. PTGaAs is the first example of a lithographically patterned quasi-phase-matched (QPM) material to operate in the long-wavelength infrared. Quasi-phase-matched materials are microstructured to allow them to efficiently phase-match nonlinear optical mixing processes (such as frequency doubling or difference frequency generation).

The structuring creates a periodic flipping of the sign of the nonlinear susceptibility along the length of the crystal (see Figure 1). At each inversion point, accumulated phase shifts between the waves that are being mixed are corrected, allowing efficient buildup of the new wave.

In contrast, conventional birefringent phasematching requires the careful selection of crystals with appropriate

birefringent properties to ensure that phase mismatches do not occur. The ability to pattern the crystal phase-matching properties via lithography is a powerful tool because it allows the use of new materials, such as GaAs. QPM also allows the highest nonlinearity of the material and any wavelengths in its transparency range to be phase-matched. These factors result in crystals that are much more tunable and efficient than those previously available.

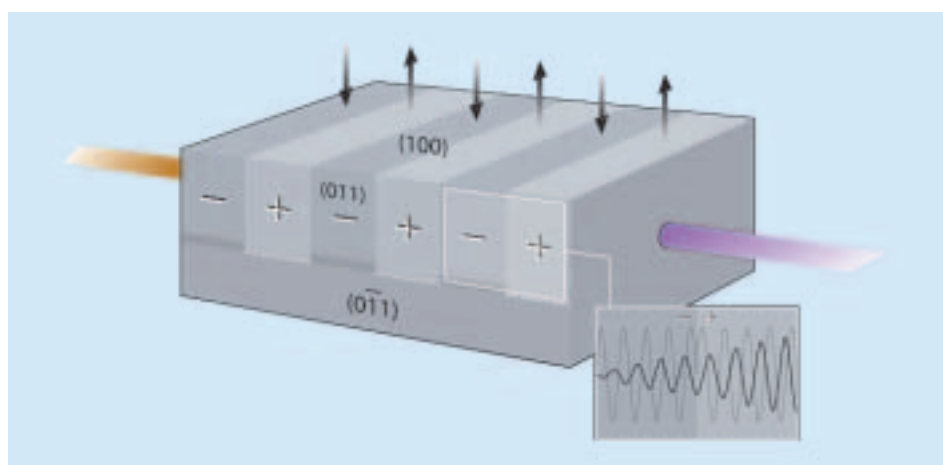


Figure 1. Enlarged view of a PTGaAs crystal. Arrows above the crystal indicate the direction of the 011 crystallographic axis. The crystals used in this work were 500- μm thick by 1.9-cm long with a 26.3- μm period. At the boundary of each domain, the phase of the generated polarization wave (the dashed line in the inset) is flipped 180°, which resynchronizes the polarization wave with the generated electric field. This is the essence of so-called quasi-phase-matching.

PTGaAs, for example, offers a nonlinear coupling 24 times greater than the birefringent material AgGaSe₂ and phasematching from 1 to 12 μm . The patterning process also allows unique spectral properties, such as the ability to temporally or spectrally shape femtosecond pulses, to be engineered into the material.

In the recent experiments, a PTGaAs crystal was used to mix light from two near-infrared diode laser sources to generate light at $\sim 7.8\ \mu\text{m}$. The apparatus used to make the measurement is shown in Figure 2. The pump sources consisted of an extended-cavity diode laser (ECDL) centered at $1.55\ \mu\text{m}$ and a distributed feedback (DFB) diode laser centered at $1.31\ \mu\text{m}$. Both are wavelengths conventionally used in the telecommunications industry. The 5-mW output of the ECDL was amplified to $\sim 1.8\ \text{W}$ by a polarization-maintaining fiber-optic amplifier prior to injection into the crystal. With a DFB output of $\sim 2\ \text{mW}$, approximately 35 nW of $7.8\ \mu\text{m}$ light were generated. Considering optical losses due to uncoated elements (including the PTGaAs) and imperfections in the crystal, this number is lower than the theoretical value by a factor of two.

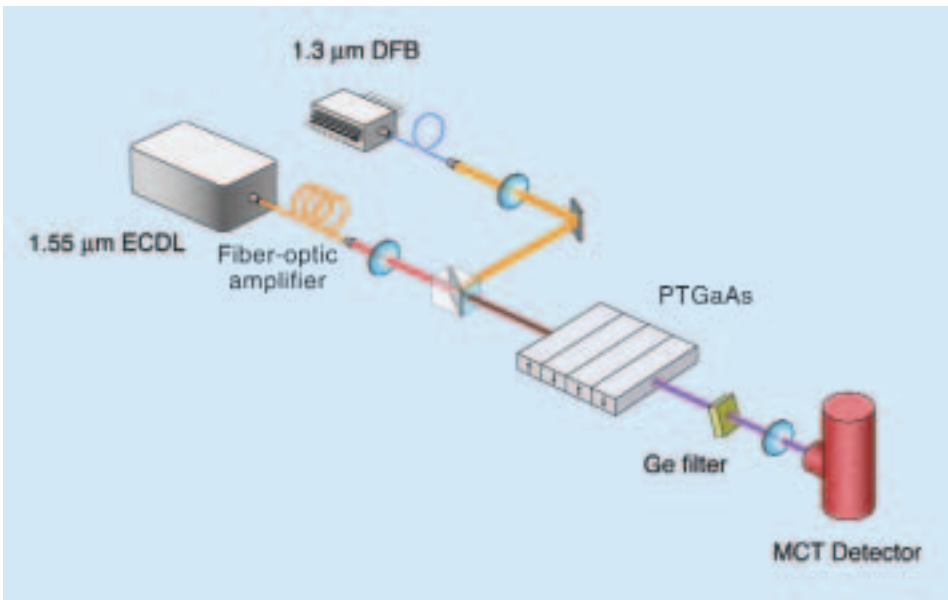


Figure 2. Schematic of the difference frequency generation (DFG) apparatus. In this work, two tunable lasers centered in the 1.3- μm and 1.5- μm telecom bands were mixed in PTGaAs to generate tunable light in the long-wave IR. Because of its engineerable properties, PTGaAs can also be used to extend the wavelength coverage of many other laser types, including ultra-short pulse lasers. The widespread use of GaAs in semiconductor devices also offers the possibility of fully integrated devices.

The performance of a PTGaAs-based source can be compared with that of quantum-cascade diode lasers (QCLs), the current state-of-the-art in LWIR spectroscopic sources. A typical DFB-QCL offers single-frequency radiation tunable over about $10\ \text{cm}^{-1}$ and requires cryogenic operation. Starting with two ECDL pump sources, tuning over $\sim 300\ \text{cm}^{-1}$ is

possible with a room temperature DFG apparatus based on PTGaAs. Although the power of the demonstrated system is low, architectures for generating 0.5 to 1 mW are possible, based on extrapolation. Ultimately, integrated devices may be possible, in which PTGaAs waveguides are coupled directly with diode pump sources on a single GaAs substrate.

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Sandia National Laboratories
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